6-Chloro-N^2-ethyl-N^4-propyl-1,3,5-triazine-2,4-diamine

90952-64-0 | DTXSID60536638

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		**Training (75%)**		**Test (25%)**	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.69e-07 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.03e-01

Confidence level: 5.92e-01

Nearest Neighbors from the Training Set

Image not found
2,4-Dinitrotoluene
Measured: 2.21e-08
Predicted: 2.66e-04

Image not found
Chlorothalonil
Measured: 2.89e-07
Predicted: 1.44e-06

Image not found
Terbacil
Measured: 1.12e-06
Predicted: 9.25e-07

Image not found
Fluopropanate-sodium
Measured: 3.00e-07
Predicted: 1.25e-02

Image not found
Limonene
Measured: 1.31e-07
Predicted: 1.32

Image not found
D-Limonene
Measured: 1.31e-07
Predicted: 1.32

Image not found
(S)-Limonene
Measured: 1.31e-07
Predicted: 1.32